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(1*Z*)-1-(4-Methoxyphenyl)ethan-1-one thiosemicarbazone

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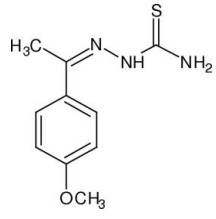
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.008 Å; R factor = 0.079; wR factor = 0.240; data-to-parameter ratio = 15.9.

Geometric parameters of the title compound, $C_{10}H_{13}N_3OS$, are in the usual ranges. There are two similar molecules (r.m.s. deviation 0.131 Å for all non-H atoms) in the asymmetric unit. The crystal packing is characterized by sheets in the (202) plane. The molecules in the sheets are connected by N—H···O and N—H···S hydrogen bonds.

Related literature

For related literature, see: Castro *et al.* (2003); Chattopadhyay *et al.* (1988); Dinçer *et al.* (2005); Kearney *et al.* (1998); Nie *et al.* (2004); Onderwater *et al.* (2004); Ren *et al.* (2000); Rodriguez-Fernandez *et al.* (2005); Sarojini *et al.* (2007); Stankovic & Vukovic (1996); Trochimczuk & Kolarz (2000); Yathirajan *et al.* (2006); Zhou *et al.* (2003).



Experimental

Crystal data

$C_{10}H_{13}N_3OS$
M_r = 223.29
Monoclinic, $P2_1/c$
a = 14.3548 (9) Å
b = 8.4141 (5) Å
c = 19.6562 (13) Å
β = 108.123 (5)°
V = 2256.4 (3) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 173 (2) K
0.31 × 0.25 × 0.18 mm

Data collection

Stoe IPDSII two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2003; Blessing, 1995)
T_{min} = 0.923, T_{max} = 0.954
42568 measured reflections
4478 independent reflections
3571 reflections with $I > 2\sigma(I)$
R_{int} = 0.082

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.079
$wR(F^2)$ = 0.240
S = 1.06
4478 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.48 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···S1^{i}	0.88	2.73	3.472 (4)	143
N3—H3A···O1A^{ii}	0.88	2.26	2.942 (5)	135
N3—H3B···S1^{iii}	0.88	2.54	3.355 (5)	154
N2A—H2N···S1A^{iv}	0.88	2.79	3.521 (4)	142
N3A—H3A1···O1^{v}	0.88	2.21	2.927 (6)	138
N3A—H3A2···S1A^{vi}	0.88	2.50	3.370 (5)	169

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $-x+1, -y+1, -z+1$; (iii) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $-x, y+\frac{1}{2}, -z+\frac{3}{2}$; (v) $-x+1, -y, -z+1$; (vi) $-x, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* in *SHELXTL-Plus* (Sheldrick, 1991); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2375).

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supplementary materials

Acta Cryst. (2007). E**63**, o4834-o4835 [**doi:10.1107/S1600536807059788**]

(1*Z*)-1-(4-Methoxyphenyl)ethan-1-one thiosemicarbazone

B. Narayana, K. Sunil, B. K. Sarojini, H. S. Yathirajan and M. Bolte

Comment

Thiourea and its derivatives have been the focus of attention in recent years in view of their interesting physicochemical properties and broad range of applications in several chemical disciplines. Certain thiourea molecules have antiviral activity and might be characterized as prospective inhibitors of many enzymes, particularly, HIV-1 reverse transcriptase (Ren *et al.*, 2000; Onderwater *et al.*, 2004). As antibacterial and antifungal agents, they have been used in agriculture (Rodriguez-Fernandez *et al.*, 2005). In technical applications, dithioamide compounds are known to be prospective nonlinear optical materials (Zhou *et al.*, 2003), corrosion inhibitors for copper and iron in acidic media (Stankovic & Vukovic 1996) and functionalization agents for production of chemically modified resins (Trochimczuk & Kolarz 2000). Thiourea derivatives have been also reported as potential receptors and ionophores for heavy metal cations (Castro *et al.*, 2003), building blocks in the synthesis of heterocyclic compounds (Kearney *et al.*, 1998). Finally, the strong hydrogen-bonding donor capability of the –N(H)—C(=S)—N(H)- group has been widely exploited in supramolecular chemistry, where it has been used as a building block for anion receptors (Nie *et al.*, 2004). The crystal structures of 1-(2-bromo-5-methoxybenzoyl)thiosemicarbazide, (Sarojini *et al.*, 2007), salicylaldehyde thiosemicarbazone (Chattopadhyay *et al.*, 1988), 4-(methylsulfanyl)benzaldehyde thiosemicarbazone (Yathirajan *et al.*, 2006) and benzoin thiosemicarbazone (Dinçer *et al.*, 2005) A new carbothioamide, (I), $C_{10}H_{13}N_3OS$, has been synthesized and its crystal structure is reported.

Geometric parameters of the title compound are in the usual ranges. There are two similar (r.m.s. deviation 0.131Å for all non-H atoms) molecules in the asymmetric unit. The crystal packing is characterized by sheets in the (202) plane. The molecules in a sheet are connected by N—H···O and N—H···S hydrogen bonds.

Experimental

A mixture of 1-(4-methoxyphenyl)ethanone (1.5 g, 0.01 mol) and hydrazinecarbothioamide (0.91 g, 0.01 mol) in 15 ml of absolute ethanol containing 2 drops of 4 *M* sulfuric acid was refluxed for about 3 h. On cooling, the solid separated was filtered and recrystallized from ethyl acetate (m.p.: 448–450 K). Analysis found: C 53.70, H 5.83, N 18.76, S 14.31%; $C_{10}H_{13}N_3OS$ requires: C 53.79, H 5.87, N 18.82, S 14.36%.

Refinement

H atoms were found in a difference map, but they were geometrically positioned and refined with fixed individual displacement parameters [U(H) = 1.2 U_{eq}(C) or U(H) = 1.5 U_{eq}(C_{methyl})] using a riding model with $C_{aromatic}$—H = 0.95 Å, C_{methyl}—H = 0.98Å and N—H = 0.88 Å The methyl groups were allowed to rotate but not to tip. The crystal was a non-merohedral twin (twin law −1 0 0/0 − 1 0/0.85 0 1) with a contribution of 66.3 (3)% of the main component.

Figures

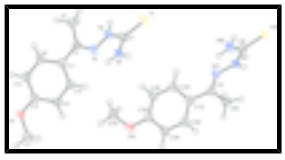


Fig. 1. Perspective view of the title compound with the atom numbering; displacement ellipsoids are at the 50% probability level.

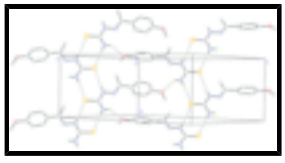


Fig. 2. Partial packing diagram of the title compound. View onto the (202) plane. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding are omitted.

(1*Z*)-1-(4-Methoxyphenyl)ethan-1-one thiosemicarbazone

Crystal data

$C_{10}H_{13}N_3OS$	F_{000} = 944
M_r = 223.29	D_x = 1.315 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.3548 (9) Å	Cell parameters from 30258 reflections
b = 8.4141 (5) Å	θ = 2.8–26.2º
c = 19.6562 (13) Å	μ = 0.27 mm^{-1}
β = 108.123 (5)º	T = 173 (2) K
V = 2256.4 (3) Å^3	Plate, yellow
Z = 8	0.31 × 0.25 × 0.18 mm

Data collection

Stoe IPDSII two-circle diffractometer	4478 independent reflections
Radiation source: fine-focus sealed tube	3571 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.082
T = 173(2) K	θ_{max} = 26.3º
ω scans	θ_{min} = 2.7º
Absorption correction: multi-scan (MULABS; Spek, 2003; Blessing, 1995)	h = −17→16
T_{min} = 0.923, T_{max} = 0.954	k = −10→10
42568 measured reflections	l = −12→24

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.079	H-atom parameters constrained
$wR(F^2)$ = 0.240	$w = 1/[\sigma^2(F_o^2) + (0.1562P)^2 + 4.346P]$

	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{max} = 0.001$
4478 reflections	$\Delta\rho_{max} = 0.79$ e Å^{-3}
282 parameters	$\Delta\rho_{min} = -0.48$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Experimental. ;

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.48440 (11)	0.23608 (16)	0.76976 (8)	0.0341 (4)
O1	0.8050 (3)	0.0042 (5)	0.38379 (19)	0.0334 (9)
N1	0.6287 (3)	0.1143 (5)	0.6373 (2)	0.0310 (10)
N2	0.5907 (3)	0.1107 (5)	0.6946 (2)	0.0297 (10)
H2	0.5967	0.0253	0.7215	0.036*
N3	0.5500 (3)	0.3732 (5)	0.6715 (2)	0.0304 (10)
H3A	0.5826	0.3733	0.6403	0.036*
H3B	0.5206	0.4603	0.6789	0.036*
C1	0.6949 (4)	0.0096 (6)	0.6359 (3)	0.0247 (10)
C2	0.7407 (4)	−0.1069 (8)	0.6946 (3)	0.0395 (13)
H2A	0.7371	−0.0650	0.7402	0.06 (2)*
H2B	0.8095	−0.1235	0.6977	0.07 (2)*
H2C	0.7055	−0.2082	0.6842	0.14 (5)*
C3	0.5450 (4)	0.2403 (6)	0.7077 (3)	0.0266 (10)
C11	0.7240 (4)	0.0096 (6)	0.5701 (3)	0.0258 (10)
C12	0.6569 (4)	0.0578 (6)	0.5050 (3)	0.0274 (10)
H12	0.5933	0.0912	0.5041	0.033*
C13	0.6808 (4)	0.0583 (6)	0.4416 (3)	0.0290 (11)
H13	0.6342	0.0910	0.3980	0.035*
C14	0.7742 (4)	0.0099 (6)	0.4433 (3)	0.0277 (11)
C15	0.8419 (4)	−0.0382 (7)	0.5070 (3)	0.0302 (11)
H15	0.9055	−0.0709	0.5077	0.036*
C16	0.8172 (4)	−0.0388 (7)	0.5697 (3)	0.0279 (11)
H16	0.8641	−0.0724	0.6131	0.033*
C17	0.7387 (4)	0.0625 (8)	0.3175 (3)	0.0409 (14)

H17A	0.6813	−0.0074	0.3019	0.061*
H17B	0.7720	0.0642	0.2809	0.061*
H17C	0.7176	0.1703	0.3246	0.061*
S1A	−0.04879 (11)	0.28900 (16)	0.75014 (8)	0.0352 (4)
O1A	0.3755 (3)	0.4380 (5)	0.42642 (19)	0.0332 (9)
N1A	0.1031 (3)	0.4094 (5)	0.6234 (2)	0.0281 (9)
N2A	0.0390 (3)	0.4199 (5)	0.6636 (2)	0.0260 (9)
H2N	0.0117	0.5106	0.6690	0.031*
N3A	0.0556 (4)	0.1494 (5)	0.6767 (2)	0.0339 (10)
H3A1	0.0897	0.1504	0.6464	0.041*
H3A2	0.0448	0.0590	0.6955	0.041*
C1A	0.1091 (4)	0.5312 (6)	0.5826 (3)	0.0264 (10)
C2A	0.0463 (4)	0.6765 (6)	0.5725 (3)	0.0310 (11)
H2A1	−0.0167	0.6492	0.5790	0.07 (2)*
H2A2	0.0351	0.7183	0.5240	0.07 (2)*
H2A3	0.0794	0.7572	0.6076	0.11 (4)*
C3A	0.0204 (4)	0.2839 (6)	0.6939 (2)	0.0247 (10)
C11A	0.1823 (4)	0.5119 (6)	0.5444 (3)	0.0254 (10)
C12A	0.2609 (4)	0.4073 (6)	0.5702 (3)	0.0292 (11)
H12A	0.2697	0.3540	0.6143	0.035*
C13A	0.3268 (4)	0.3796 (6)	0.5323 (3)	0.0294 (11)
H13A	0.3799	0.3081	0.5505	0.035*
C14A	0.3143 (4)	0.4573 (6)	0.4679 (3)	0.0266 (10)
C15A	0.2370 (4)	0.5645 (7)	0.4413 (3)	0.0297 (11)
H15A	0.2290	0.6181	0.3973	0.036*
C16A	0.1721 (4)	0.5919 (7)	0.4799 (3)	0.0296 (11)
H16A	0.1201	0.6658	0.4623	0.036*
C17A	0.4539 (4)	0.3252 (6)	0.4501 (3)	0.0322 (12)
H17D	0.4976	0.3570	0.4972	0.048*
H17E	0.4909	0.3221	0.4158	0.048*
H17F	0.4268	0.2197	0.4535	0.048*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0511 (8)	0.0239 (6)	0.0392 (7)	−0.0035 (6)	0.0314 (6)	−0.0025 (5)
O1	0.034 (2)	0.041 (2)	0.0301 (18)	0.0052 (16)	0.0170 (16)	0.0016 (16)
N1	0.039 (2)	0.028 (2)	0.032 (2)	−0.0009 (19)	0.020 (2)	−0.0008 (18)
N2	0.045 (3)	0.022 (2)	0.030 (2)	0.0007 (19)	0.023 (2)	0.0026 (17)
N3	0.043 (3)	0.028 (2)	0.027 (2)	0.001 (2)	0.022 (2)	−0.0018 (18)
C1	0.023 (2)	0.024 (2)	0.027 (2)	−0.0009 (19)	0.0091 (19)	0.0019 (19)
C2	0.042 (3)	0.049 (3)	0.029 (3)	0.014 (3)	0.012 (2)	0.009 (3)
C3	0.033 (3)	0.024 (2)	0.025 (2)	−0.006 (2)	0.013 (2)	−0.0031 (19)
C11	0.031 (3)	0.019 (2)	0.029 (2)	0.0030 (19)	0.012 (2)	0.0005 (19)
C12	0.025 (2)	0.029 (3)	0.029 (2)	0.005 (2)	0.010 (2)	0.002 (2)
C13	0.030 (3)	0.030 (3)	0.027 (2)	0.004 (2)	0.009 (2)	0.002 (2)
C14	0.034 (3)	0.025 (3)	0.029 (2)	0.000 (2)	0.016 (2)	0.000 (2)
C15	0.026 (3)	0.033 (3)	0.034 (3)	0.002 (2)	0.012 (2)	0.000 (2)

C16	0.023 (2)	0.033 (3)	0.027 (2)	0.006 (2)	0.007 (2)	0.004 (2)
C17	0.041 (3)	0.055 (4)	0.028 (3)	0.005 (3)	0.013 (2)	0.007 (3)
S1A	0.0495 (8)	0.0254 (6)	0.0436 (8)	−0.0024 (6)	0.0331 (7)	−0.0012 (5)
O1A	0.036 (2)	0.037 (2)	0.0314 (18)	0.0035 (17)	0.0180 (17)	0.0046 (16)
N1A	0.033 (2)	0.027 (2)	0.030 (2)	0.0015 (18)	0.0175 (19)	0.0035 (17)
N2A	0.035 (2)	0.0195 (19)	0.029 (2)	0.0019 (17)	0.0177 (19)	0.0037 (16)
N3A	0.051 (3)	0.023 (2)	0.037 (2)	−0.005 (2)	0.027 (2)	−0.0012 (19)
C1A	0.030 (3)	0.024 (2)	0.024 (2)	−0.001 (2)	0.007 (2)	−0.0010 (19)
C2A	0.040 (3)	0.025 (3)	0.035 (3)	0.005 (2)	0.021 (2)	0.003 (2)
C3A	0.029 (2)	0.022 (2)	0.024 (2)	−0.004 (2)	0.010 (2)	−0.0012 (18)
C11A	0.030 (3)	0.021 (2)	0.026 (2)	−0.0071 (19)	0.011 (2)	−0.0039 (18)
C12A	0.034 (3)	0.030 (3)	0.024 (2)	0.000 (2)	0.009 (2)	0.004 (2)
C13A	0.031 (3)	0.031 (3)	0.030 (2)	0.004 (2)	0.014 (2)	0.005 (2)
C14A	0.030 (3)	0.024 (2)	0.028 (2)	−0.003 (2)	0.013 (2)	−0.003 (2)
C15A	0.030 (3)	0.035 (3)	0.026 (2)	−0.004 (2)	0.012 (2)	0.001 (2)
C16A	0.031 (3)	0.030 (3)	0.029 (3)	−0.002 (2)	0.012 (2)	0.000 (2)
C17A	0.032 (3)	0.028 (3)	0.040 (3)	0.001 (2)	0.016 (2)	−0.001 (2)

Geometric parameters (Å, °)

S1—C3	1.704 (5)	S1A—C3A	1.701 (5)
O1—C14	1.374 (6)	O1A—C14A	1.381 (6)
O1—C17	1.439 (7)	O1A—C17A	1.434 (6)
N1—C1	1.302 (6)	N1A—C1A	1.320 (7)
N1—N2	1.398 (6)	N1A—N2A	1.389 (6)
N2—C3	1.338 (6)	N2A—C3A	1.354 (6)
N2—H2	0.8800	N2A—H2N	0.8800
N3—C3	1.339 (7)	N3A—C3A	1.326 (7)
N3—H3A	0.8800	N3A—H3A1	0.8800
N3—H3B	0.8800	N3A—H3A2	0.8800
C1—C11	1.478 (7)	C1A—C11A	1.478 (7)
C1—C2	1.500 (7)	C1A—C2A	1.495 (7)
C2—H2A	0.9800	C2A—H2A1	0.9800
C2—H2B	0.9800	C2A—H2A2	0.9800
C2—H2C	0.9800	C2A—H2A3	0.9800
C11—C12	1.401 (7)	C11A—C12A	1.397 (7)
C11—C16	1.401 (7)	C11A—C16A	1.402 (7)
C12—C13	1.391 (7)	C12A—C13A	1.393 (7)
C12—H12	0.9500	C12A—H12A	0.9500
C13—C14	1.391 (7)	C13A—C14A	1.387 (7)
C13—H13	0.9500	C13A—H13A	0.9500
C14—C15	1.386 (8)	C14A—C15A	1.398 (8)
C15—C16	1.384 (7)	C15A—C16A	1.393 (7)
C15—H15	0.9500	C15A—H15A	0.9500
C16—H16	0.9500	C16A—H16A	0.9500
C17—H17A	0.9800	C17A—H17D	0.9800
C17—H17B	0.9800	C17A—H17E	0.9800
C17—H17C	0.9800	C17A—H17F	0.9800
C14—O1—C17	117.4 (4)	C14A—O1A—C17A	117.7 (4)

C1—N1—N2	118.2 (4)	C1A—N1A—N2A	118.4 (4)
C3—N2—N1	118.4 (4)	C3A—N2A—N1A	116.9 (4)
C3—N2—H2	120.8	C3A—N2A—H2N	121.6
N1—N2—H2	120.8	N1A—N2A—H2N	121.6
C3—N3—H3A	120.0	C3A—N3A—H3A1	120.0
C3—N3—H3B	120.0	C3A—N3A—H3A2	120.0
H3A—N3—H3B	120.0	H3A1—N3A—H3A2	120.0
N1—C1—C11	115.1 (4)	N1A—C1A—C11A	114.5 (4)
N1—C1—C2	125.1 (5)	N1A—C1A—C2A	124.4 (5)
C11—C1—C2	119.8 (4)	C11A—C1A—C2A	121.1 (4)
C1—C2—H2A	109.5	C1A—C2A—H2A1	109.5
C1—C2—H2B	109.5	C1A—C2A—H2A2	109.5
H2A—C2—H2B	109.5	H2A1—C2A—H2A2	109.5
C1—C2—H2C	109.5	C1A—C2A—H2A3	109.5
H2A—C2—H2C	109.5	H2A1—C2A—H2A3	109.5
H2B—C2—H2C	109.5	H2A2—C2A—H2A3	109.5
N2—C3—N3	117.9 (4)	N3A—C3A—N2A	117.8 (4)
N2—C3—S1	120.7 (4)	N3A—C3A—S1A	122.2 (4)
N3—C3—S1	121.4 (4)	N2A—C3A—S1A	120.0 (4)
C12—C11—C16	117.7 (5)	C12A—C11A—C16A	118.4 (5)
C12—C11—C1	119.9 (5)	C12A—C11A—C1A	120.5 (4)
C16—C11—C1	122.4 (5)	C16A—C11A—C1A	121.1 (5)
C13—C12—C11	121.9 (5)	C13A—C12A—C11A	121.2 (5)
C13—C12—H12	119.1	C13A—C12A—H12A	119.4
C11—C12—H12	119.1	C11A—C12A—H12A	119.4
C12—C13—C14	118.8 (5)	C14A—C13A—C12A	119.5 (5)
C12—C13—H13	120.6	C14A—C13A—H13A	120.2
C14—C13—H13	120.6	C12A—C13A—H13A	120.2
O1—C14—C15	116.0 (5)	O1A—C14A—C13A	123.9 (5)
O1—C14—C13	123.6 (5)	O1A—C14A—C15A	115.6 (4)
C15—C14—C13	120.4 (5)	C13A—C14A—C15A	120.5 (5)
C16—C15—C14	120.3 (5)	C16A—C15A—C14A	119.4 (5)
C16—C15—H15	119.9	C16A—C15A—H15A	120.3
C14—C15—H15	119.9	C14A—C15A—H15A	120.3
C15—C16—C11	120.9 (5)	C15A—C16A—C11A	120.9 (5)
C15—C16—H16	119.6	C15A—C16A—H16A	119.5
C11—C16—H16	119.6	C11A—C16A—H16A	119.5
O1—C17—H17A	109.5	O1A—C17A—H17D	109.5
O1—C17—H17B	109.5	O1A—C17A—H17E	109.5
H17A—C17—H17B	109.5	H17D—C17A—H17E	109.5
O1—C17—H17C	109.5	O1A—C17A—H17F	109.5
H17A—C17—H17C	109.5	H17D—C17A—H17F	109.5
H17B—C17—H17C	109.5	H17E—C17A—H17F	109.5
C1—N1—N2—C3	161.5 (5)	C1A—N1A—N2A—C3A	167.8 (5)
N2—N1—C1—C11	173.8 (4)	N2A—N1A—C1A—C11A	177.5 (4)
N2—N1—C1—C2	−5.8 (8)	N2A—N1A—C1A—C2A	−4.4 (7)
N1—N2—C3—N3	−9.0 (7)	N1A—N2A—C3A—N3A	−7.4 (7)
N1—N2—C3—S1	172.2 (4)	N1A—N2A—C3A—S1A	174.4 (3)
N1—C1—C11—C12	−28.9 (7)	N1A—C1A—C11A—C12A	−23.1 (7)

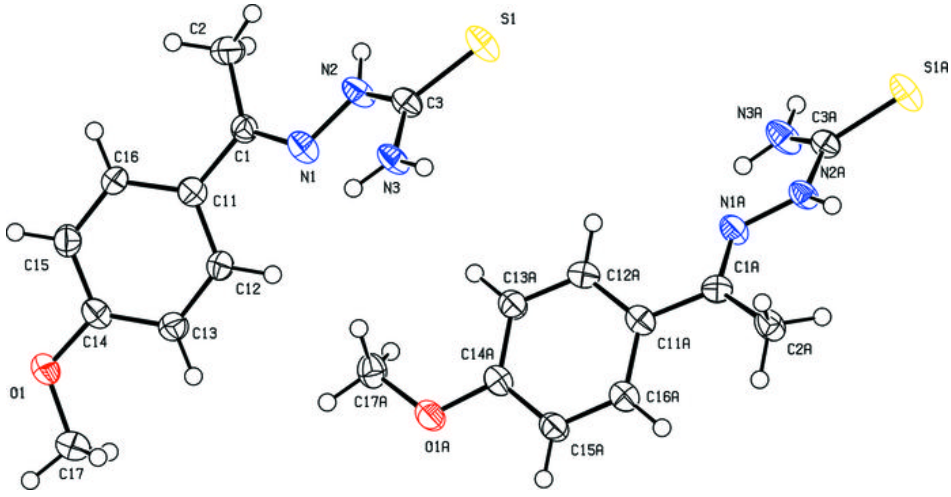
C2—C1—C11—C12	150.7 (5)	C2A—C1A—C11A—C12A	158.7 (5)
N1—C1—C11—C16	151.7 (5)	N1A—C1A—C11A—C16A	153.8 (5)
C2—C1—C11—C16	−28.7 (8)	C2A—C1A—C11A—C16A	−24.3 (7)
C16—C11—C12—C13	0.1 (8)	C16A—C11A—C12A—C13A	−1.4 (8)
C1—C11—C12—C13	−179.3 (5)	C1A—C11A—C12A—C13A	175.6 (5)
C11—C12—C13—C14	−0.3 (8)	C11A—C12A—C13A—C14A	0.0 (8)
C17—O1—C14—C15	−176.3 (5)	C17A—O1A—C14A—C13A	2.9 (7)
C17—O1—C14—C13	4.6 (8)	C17A—O1A—C14A—C15A	−177.9 (5)
C12—C13—C14—O1	179.3 (5)	C12A—C13A—C14A—O1A	−180.0 (5)
C12—C13—C14—C15	0.2 (8)	C12A—C13A—C14A—C15A	0.9 (8)
O1—C14—C15—C16	−179.1 (5)	O1A—C14A—C15A—C16A	−179.7 (5)
C13—C14—C15—C16	0.1 (8)	C13A—C14A—C15A—C16A	−0.5 (8)
C14—C15—C16—C11	−0.3 (8)	C14A—C15A—C16A—C11A	−0.9 (8)
C12—C11—C16—C15	0.2 (8)	C12A—C11A—C16A—C15A	1.8 (8)
C1—C11—C16—C15	179.6 (5)	C1A—C11A—C16A—C15A	−175.2 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···S1^{i}	0.88	2.73	3.472 (4)	143
N3—H3A···O1A^{ii}	0.88	2.26	2.942 (5)	135
N3—H3B···S1^{iii}	0.88	2.54	3.355 (5)	154
N2A—H2N···S1A^{iv}	0.88	2.79	3.521 (4)	142
N3A—H3A1···O1^{v}	0.88	2.21	2.927 (6)	138
N3A—H3A2···S1A^{vi}	0.88	2.50	3.370 (5)	169

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+3/2; (ii) −*x*+1, −*y*+1, −*z*+1; (iii) −*x*+1, *y*+1/2, −*z*+3/2; (iv) −*x*, *y*+1/2, −*z*+3/2; (v) −*x*+1, −*y*, −*z*+1; (vi) −*x*, *y*−1/2, −*z*+3/2.

Fig. 1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C3
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C3A
C16
C1
N1
N3
N2A
C11
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C12
C13A
C12A
C1A
C14
C13
C11A
C2A
C14A
O1
C17A
C16A
O1A
C15A
C17

Fig. 2